#### Geothermal Technologies Office 2013 Peer Review

**ENERGY** Energy Renewa

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An integrated experimental and numerical study: Developing a reaction transport model that couples chemical reactions of mineral dissolution / precipitation with spatial and temporal flow variations in  $CO_2$ /brine/rock systems

Total Project Funding: \$1,937,523 (\$1,550,018 from DOE-GTP) April 23, 2013, 9:30-10:00am

This presentation does not contain any proprietary confidential, or otherwise restricted information.

R&D Project Supercritical CO<sub>2</sub> / Rock Chemical Interactions

#### Principal Investigator: Martin Saar Department of Earth Sciences University of Minnesota

Track Name: Resource Characterization, Modeling, Supercritical CO<sub>2</sub> / Rock Chemical Interactions

### Relevance/Impact of Research Weight: 20%



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**General Research Topic/Goal and impact on GTP's goals:** This project applies to the DOE Geothermal Technologies Program's Multi-Year Research, Develop-ment, and Demonstration (MYRDD) plan as the research would further the development and commercial operation of an enhanced geothermal system (EGS) resource through investigation of Topic 14 of FOA DE-PS36-09GO99018. In particular, the proposed study would address issues related to geothermal reservoir sustainability. The goal of "Reservoir Sustainability," as outlined in MYRDD's Technical Plan, is to "Develop the ability to manage EGS reservoirs for maintenance of reservoir lifetime and productivity." Our proposed study would address the two tasks listed in Table 4.29 (Page 75) of MYRDD's "Reservoir Sustainability" section, i.e., "Stimulation and management of created reservoir" and "Maintaining fluid flow and reservoir lifetime." These tasks would be achieved via the approach listed in Table 4.29 entitled "Improve understanding of rock-fluid geochemistry for scale and dissolution prediction."

**Project Outcome:** This project will result in a numerical simulator (modified version of TOUGH2) that can adjust porosity and permeability fields according to experimentally observed chemical fluid-rock interactions (mineral dissolution or precipitation) under realistic conditions likely found when water or (supercritical) CO<sub>2</sub> is injected into geothermal reservoirs for heat energy extraction.

**Relevance/Impact:** The simulator can thus help determine if  $CO_2$  injection into EGS brines will cause clogging of pore spaces or dissolution of host rocks with potentially detrimental consequences to heat extraction. As a result, this simulator will play a critical role when assessing long-term sustainability of geothermal energy utilization in enhanced and natural geothermal systems. The simulator can also be used to evaluate long-term  $CO_2$  sequestration potentials.





### Scientific/Technical Approach Weight: 30%

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#### Task 1 Experiment:

**Schematic of fluid flow and reaction cell system -** chemical monitoring of complex fluid-mineral reactions at elevated T, P, and CO<sub>2</sub>.





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### Scientific/Technical Approach Weight: 30%





### **Tomographic Particle Image Velocimetry (TPIV) setup**

- 1) Sequences of fluid motion (e.g. interface, bulk drop) are captured at high repetition rate using high speed cameras.
- 2) Temporal deformation of interface or drop under different conditions can be compared with results from LB code.
- Time series of volumetric velocity fields are acquired using 3D tomographic PIV (TPIV).
- Velocity obtained simultaneously in two immiscible fluids by matching refractive indices (likely 1<sup>st</sup> time as TPIV worldwide).





 -Use PIV and analog fluids to test LB code (then use LB code to run simulations with CO<sub>2</sub> and brine)



Fluid II

Solid

### Scientific/Technical Approach Weight: 30%

### Task 4 LB:

# Lattice-Boltzmann (LB) Simulations – extending/modifying our in-house LB code: LBHydra<sup>TM</sup> (lbhydra.umn.edu)

LB methods are bottom-up methods where microscopic fluid and solute packages interact, allowing detailed simulations of macroscopic multiphase multicomponent fluid flow and heat transfer and fluid-mineral reactions within porous/fractured media without requiring a-priori knowledge of permeability, k, tensor fields. Thus, LB methods can be used as numerical permeameters, allowing determination of k fields which complements lab bulk sample k determinations. In addition, the LB simulations provide the fluid flow field, complementing X-ray computed tomography (XRCT) information of the solid phase. XRCT data serves as input to LB models.

2 panels to the right: Walsh et al., 2009



#### From the LBHydra<sup>™</sup> home page at: Ibhydra.umn.edu

LBHydra

QUICKSTART MANUAL PUBLICATIONS SUPPORT LINKS



#### Lattice Boltzmann simulation package

LBHydra is a modular, extensible Lattice-Boltzmann simulation package capable of modeling a wide array of fluid mechanical behavior. The Lattice-Boltzmann methods provided with LBHydra are capable of simulating laminar and turbulent flows, heat and mass transport, and multiple phase and multiple component fluids in complex and changing fluid flow geometries.

The simulation engine offers numerous areas for user input and modification, including user-defined material modules, lattice-types and subroutines, thus enabling far more complex simulations. Furthering the benefit of modularity is the ability to couple LBHydra with other applications, either by linking to the simulation engine directly or by employing LBHydra's libraries within an application.

Additional modules provided with the simulator allow the user to harness the power of CUDA-compliant nVIDIA graphics processing units (GPUs). These modules transfer the calculation from CPU to GPU, with the potential to accelerate simulations up to 40x faster.

#### Licensing

The beta version of LBHydra is now available without charge for academic users. Visit LBHydra's page with the Office for Technology Commercialization at the University of Minnesota for details on licensing agreements and obtaining a copy of the package.



Fig. 1. Part of a two-dimensional (D2Q9) lattice-Boltzmann lattice (a). Fluid packets are propagated between nodes during streaming steps (b) and redirected during collision steps (c).









Images from LBHydra simulations: i. Droplets form in an immiscible fluid mixture. ii. Fluid flow through a pumice sample. iii. Phase separation.

LBHydra<sup>™</sup> runs on multiple Graphics Processing Units (GPUs), each with hundreds of simple but sufficient processors. This unique capability of our LB code makes it possible to run the required single- and multi-phase simulations of CO<sub>2</sub> and water or brine flow within a porous medium in a reasonable amount of time (hours as opposed to days or weeks). This GPU implementation of an LB code is an active research project of the PI and constitutes a significant and critical contribution to this DOE project.

#### Weight: 40%



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Weight: 40%

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### Tasks 1 & 2 Exp., XRCT

### **Reactive flow-through experiments and X-Ray Computed Tomography (XRCT) before and after experiments**



Basalt core drilled from a piece of Columbia River Basalt collected in Washington. XRCT scans before and after flow-though carbon seguestration experiments are used to document changes in pore space geometries produced by mineral dissolution and/or precipitation. Sample size is approximately 0.5 in X 1 in.

Figure below: Dissolution channel developed in dolostone core exposed to flowing brine with dissolved CO<sub>2</sub>. Yellow dissolution channel illustrates the network of connected pore space mapped using post-experiment XRCT scans. One molal NaCl brine with a CO<sub>2</sub> concentration of 0.6 mol/kg H2O flows from left to right. Core is 1.3 cm in diameter and 2.5 cm long. The dissolution channel penetrated 1.4 cm of the core's length over 6.1 hours of fluid flow through the core. Permeability was measured with increasing from 4.3 × 10-16 m2 to 1.4 × 10-15 m2 because of the development of a dissolution channel. Pre- and post-experiment XRCT scans were used to show that pore volume increased from 139.0 mm<sup>3</sup> to 212.1 mm<sup>3</sup>, pore surface area increased 0.0200 m<sup>2</sup> from to 0.0224 m<sup>2</sup>, porosity increased from 5.75% to 6.37%, and specific surface area (pore surface area to pore volume) decreased from 1.436 × 105 m<sup>-1</sup> to 1.057 × 105 m<sup>-1</sup>.



**Dissolution Channel** Determined from Before XRCT images From before and after Reactive flow.

Figure below: Permeability, k, fields are numerically determined by numerical simulations of equilibrium fluid flows through the dolostone samples using lattice-Boltzmann method. (a) Permeability fields (in m<sup>2</sup>) of a Representative Elementary Volume (REV) along the connected channel of the dolostone sample. This REV has a size of around  $1 \times 1 \times 1$  mm<sup>3</sup>, which is a portion of the connected channel from Fig.1 (b). The velocity field at equilibrium status of a micro-channel in the sub-REV scale, which has a size of 200 x 120 x 80 µm<sup>3</sup>.





One Representative **Elementary Volume** (REV).

### Weight: 40%

Tasks 1 & 2

Exp., XRCT

Initial *k*: 3.8

Final *k*: 1.8

Initial k: 4.3

Final *k*: 1.4

Initial k: 3.5

Final *k*: 3.1

### **Reactive flow-through experiments and X-Ray Computed Tomography (XRCT) before and after experiments**

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Arkose

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Luhmann, A.J., X.-Z. Kong, B.M. Tutolo, K. Ding, M.O. Saar, and W.E. Seyfried, Jr. 2012. Permeability reduction produced by grain reorganization and accumulation of exsolved CO<sub>2</sub> during geologic carbon sequestration: A new CO<sub>2</sub> trapping mechanism. Environmental Science & Technology. 47(1):242-251.

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#### eere.energy.gov

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Analog for CO<sub>2</sub> drop (nonwetting) displacing brine

Bordoloi, A., Longmire, E.K. 2012. Effects of surface wettability and edge geometry on drop motion through an orifice. Am. Phys. Soc. Meeting, 2012. Bordoloi, A.D. and Longmire, E.K. 2012. Effect of neighboring perturbations on drop coalescence at an interface. Physics of Fluids. 24(062106):1-21.

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### Weight: 40%



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#### Weight: 40%

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Original Planned Milestone/Technical Accomplishment	Actual Milestone/Technical Accomplishment	Date Completed
Task 1:Laboratoryexperiments with supercriticalCO2, brine, rock. Measure fluidchemistry and bulkrock/sediment permeabilitychange over timeTask 1 is scheduled to occurthroughout the grant duration.Task 2:X-Ray ComputedTomography (XRCT) beforeand after experiments→ Measure 3D pore spacegeometry change due tomineral/fluid reactionsTask 2:scheduled to occurthroughout the grant duration.Task 3:PIV experiments ofmultiphase fluid flow andinteractions with solidboundaries to validate LB codeTask 4:Extend lattice-Boltzmann (LB) fluid flowcode (LBHydra) and use 3DXRCT images in simulations	<ul> <li>Luhmann, A.J., XZ. Kong, B.M. Tutolo, K. Ding, M.O. Saar, and W.E. Seyfried, Jr. 2012. Permeability reduction produced by grain reorganization and accumulation of exsolved CO<sub>2</sub> during geologic carbon sequestration: A new CO<sub>2</sub> trapping mechanism. Environmental Science &amp; Technology. 47(1):242-251.</li> <li>Luhmann, A.J., XZ. Kong, B.M. Tutolo, M.O. Saar, and W.E. Seyfried, Jr. 2012. Physical and chemical processes affecting permeability during geologic carbon sequestration in arkose and dolostone: Experimental observations. Abstract H32A-07. Fall Meeting, AGU, 2012.</li> <li>Kong, XZ., B.M. Tutolo, A.J. Luhmann, M.O. Saar, and W.E. Seyfried, Jr. 2012. Characterization of permeability fields and fluid flow through rock core during CO<sub>2</sub> sequestration. Abstract H23E-1422. 2012 Fall Meeting, AGU, 2012.</li> <li>Tutolo, B.M., A.J. Luhmann, XZ. Kong, M.O. Saar, and W.E. Seyfried, Jr. 2012. Linking pore-scale chemical processes to continuum-scale flow properties: an experimental and theoretical reactive transport approach. Abstract H23E-1425. Fall Meeting, AGU, 2012.</li> <li>Luhmann, A.J., R.M. Tutolo, XZ. Kong, M.O. Saar, and W.E. Seyfried, Jr. 2012. Permeability change from CO<sub>2</sub> injection: Experimental considerations. 2012 Goldschmidt Meeting, Montreal, Canada, 2012.</li> <li>Tutolo, B.M., A.J. Luhmann, XZ. Kong, M.O. Saar, and W.E. Seyfried, Jr. 2012. Evaluating permeability change due to altered pore geometry in CO<sub>2</sub> sequestration systems. 2012 Goldschmidt Meeting, Canada, 2012.</li> <li>Kong, X. and M.O. Saar and W.E. Seyfried, Jr. 2011. Evaluating permeability change due to altered pore geometry in CO<sub>2</sub> sequestration systems. 2012 Goldschmidt Meeting, Montreal, Canada, 2012.</li> <li>Kong, X. and M.O. Saar and W.E. Seyfried, Jr. 2011. Effects of small-scale chemical reactions between supercritical CO<sub>2</sub> and arkosic sandstone on large-scale permeability fields: An experimental study with implications for geologic carbon sequestration. Abstract H516-1261. A</li></ul>	See dates of publications + work is ongoing
Task 5: TOUGH2 simulations, Parameterize permeability changes due to reactive flow experiments, Thermodynamic data base assessment	<ul> <li>Tutolo B.M., XZ. Kong, W.E. Seyfried Jr., and M.O. Saar, Evaluation and revision of Aluminum Mineral Thermodynamic Data for aqueous geochemical applications, Geochimica et Cosmochimica Acta, in review, 2012 / 2013.</li> <li>Kong, Xiang-Zhao, B.M. Tutolo, and M.O. Saar. 2013. DBCreate: A SUPCRT92-based Program for Producing EQ3/6, TOUGHREACT, and GWB Thermodynamic Databases at user-defined T and P. Computers &amp; Geosciences. 51:415-417.</li> <li>Kong, X. and M.O. Saar. 2011. Effects of permeability heterogeneity on density-driven convection during CO<sub>2</sub> dissolution storage in saline aquifers. Abstract H21C-1121. AGU 2011 Fall Meeting, San Francisco, CA.</li> <li>Tutolo, B.M., W.E. Seyfried and M.O. Saar. 2011. An assessment of thermodynamic database effects on reactive transport models' predictions of permeability fields. Abstract H51C-1216. AGU 2011 Fall Meeting, San Francisco, CA.</li> <li>Randolph, J.B., and M.O. Saar. 2011. Combining geothermal energy capture with geologic carbon dioxide sequestration. Geophysical Research Letters. 38(L10401):1-7.</li> <li>Randolph, J.B. and M.O. Saar. 2011. Coupling carbon dioxide sequestration with geothermal energy capture in naturally permeable, porous geologic formations: Implications for CO<sub>2</sub> sequestration. Energy Procedia. 4:2206-2213. DOI: 10.1016/j.egypro.2011.02.108.</li> </ul>	See dates of publications + work is ongoing

#### Mandatory- may utilize multiple slides

# Project Management/Coordination Future Directions Weight: 10%

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Describe deployment strategy or expected outcome of this effort. Discuss future research, development or deployment needs.

- Explain key activities for the rest of FY2013 and to project completion.
- Be as specific as possible; avoid blanket statements.
- Address how you will deal with any decision points during that time and any remaining issues, including any alternative development pathways under consideration to mitigate risk of not achieving milestones.
- The project is on track and should finish by the end date of 9/30/2013 (~6 months from now).
- An NSF proposal has been submitted in January 2013 to continue this type of research by conducting in-situ XRCT experiments to allow for higher temporal resolution time series experiments of reactive transport. This would improve our understanding of how mineral dissolution or precipitation affect permeabilities during geologic CO<sub>2</sub> sequestration and/or usage of CO<sub>2</sub> as a working fluid during geothermal heat energy extraction.

Include the planned milestones and go/no-go decisions for FY13 and beyond and current status of working towards them. You may utilize the table below for this purpose. If this is different from your original plan, please explain why.

 The project has no go/no-go decision points or specific milestones to be reached before the expected project completion date. The project is on track and should come to completion by the expected completion date of 9/30/2013 if no further complications arise.

The project is progressing well and is entering its final phase. Portions of tasks 1-4 are still in progress and Task 5 has now also been entered during which results from Tasks 1-4 will be integrated. Thus all 5 tasks are progressing well and work will continue throughout the remainder of the project which has a current end date of 9/30/2013.

**Task 1:** We have run dolostone and arkose reactive flow-through experiments and will continue with a few more. We have had difficulty finding basalts with sufficient initial permeability but now have working samples. This will complete Task 1.

Task 2: XRCT 3D imaging is ongoing before and after each experiment from Task 1.

Task 3: PIV experiments are ongoing to test the LB fluid flow simulator (Task 4)

**Task 4:** The LB code has been extended and is being used to determine permeability fields of XRCT determined 3D pore structure of representative elementary volumes (REVs) with one permeability value for each REV.

**Task 5:** We have started to run TOUGH2 simulations of  $CO_2$ /water/brine flow and heat transfer. Simulations and are now beginning to use the results from Tasks 1-4 to integrate the information on how reactions, due to  $CO_2$ /water/mineral reactions, affect permeability fields, to include in parameterized form, for various rock types, temperatures, and pressures into TOUGH2.



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### The project is progressing well and is on schedule.

#### The following accomplishments have been made to date (March 2013):

- We have conducted reactive flow-through experiments with carbonates (dolostone) and arkose sandstones and have started experiments with basalts that show high-enough initial permeability for experiments. (Task 1)
- We have installed and tested our in-house X-Ray Tomography (XRCT) system in the spring of 2012 and conducted before and after (experiment) 3D imaging of rocks at this facility and in since 2011 at Argonne National Lab. (Task 2)
- We have conducted Particle Image Velocimetry (PIV) experiments of multiphase (analogue) fluid flow through simple porous media (orifice plate) as well as drop collapse PIV experiments to test our in-house LB code. (Task 3)
- We have run lattice-Boltzmann (LB) multiphase fluid flow simulations of the PIV experiments and of fluid flow through XRCT-determined 3D pore spaces of our actual samples to determine permeability fields and their changes (due to reactions) of the reactive flow experiments. These simulations help parameterization of permeability changes due to reactive transport as observed in the physical experiments which will be integrated into TOUGH2. (Task 1-4)
- We have run TOUGH2 simulations of water/brine and dissolved CO<sub>2</sub> to investigate CO<sub>2</sub> dissolution (in brine) storage with implications for CO<sub>2</sub> plume formation and related CO<sub>2</sub>-based heat energy extraction and CO<sub>2</sub> storage capacity. (Task 5)
- We have found a new CO<sub>2</sub> storage mechanism due to exsolution of CO<sub>2</sub> out of water/brine and published the results. (Task 1-4)
- We have developed a long-overdue update of the thermodynamic data base used in aqueous geochemical modeling (e.g., in TOUGHREACT, GWB, ...) and developed software (DBCreate) for rapid inclusion of the updated data for user-defined P-T conditions (essentially resolved the so-called Aluminum problem). See publications. (Task 5)
- We have measured contact angles between CO<sub>2</sub>, water/brine, and various minerals for inclusion in LB simulations. (Tasks 1, 4) Remaining tasks (aside from finishing some of the above tasks: Tasks 1-5):
- Parameterization of how permeability changes at various P-T conditions for the investigated lithologies. (Task 5)
- Inclusion of the above parameterization into TOUGH2 so that permeability fields are adjusted during simulations based on the results of this study. **(Task 5)**

# Project Management/Coordination Project Management Weight: 10%

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- The purpose of this slide is to provide some context for evaluating your project.
- Please prepare one overview slide containing the following information:

Timeline:	Planned Start Date		Planned End Date		Actual Start Date		Current End Date	
	01/08/2010		02/28/2013		04/01/2010		09/30/2013	
Budget:	Federal Share	Cost Sh	nare	Planned Expenses to Date	Actual Expenses to Date	Valu Work Co to D	e of mpleted ate*	Funding needed to Complete Work
	\$1,550,018	\$387,5	505	\$1,520,000	\$1,410,442	\$1,49	4,000	\$527,081

\* Estimate made using the updated worksheet.

- Summarize management activities or approaches, for example:
  - Application of resources and leveraged funds/budget/spend plan
  - How is this project integrated with other projects in the Office?

Results from this project have been used to submit an NSF proposal in January 2013 that, if funded, would take the research started under this DOE grant to the next level by conducting in-situ XRCT experiments. This would allow improved (higher temporal resolution) time series analysis of how reactive transport (due to CO2 injection into deep saline aquifers during CO2 sequestration and/or CO2-based geothermal energy extraction) affects permeability field variations with implications to injectivity, CO2 storage capability, and heat extraction capability.

Coordination with industry & stakeholders

CO2-Plume Geothermal (CPG) technology has been patented by the University of Minnesota and licensed to Heat Mining Company LLC for commercialization.

• If your project is behind schedule, please tell us here.

The project is approximately on schedule and should be finished by the current expected completion date of 9/30/2013, if no further complications arise.